BASF Aktiengesellschaft

November 4, 2002 B02/0609 IB/KO/ewe

We claim:

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1. A compound of the formula Ia or Ib

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where,

in the formula Ia,

E1 is O, S, Se, Te, NR, CR2, PR,

E2, E3 are each CR, N, P,

E4 15 is N, P,

> E5 is OH, SH, NHR, or OR', SR', NRR',

E6 is NH, PH, or NR', PR',

 R^5, R^6 are each hydrogen or a linear, branched or cyclic alkyl radical or an

aryl radical,

R1, R2, R3, R4 are each hydrogen, a linear, branched or cyclic alkyl radical, an aryl 20

radical, a halogen or a nitro group,

is hydrogen, a linear, branched or cyclic alkyl radical, R

R' is a linear, branched or cyclic alkyl radical,

where at least one of the groups E5 and E6 contains a hydrogen atom;

25 in the formula Ib,

the symbols E1, E4, E5, E6, R5, R6, R1, R2, R3, R4, R and R1 are as defined in

formula Ia

and

E2' and E3' are each O, S, Se, Te, NR, CR2, PR.

- 2. A compound as claimed in claim 1, wherein E1 is S.
- 3. A compound as claimed in claim 1 or 2, wherein E4 is N.
- 4. A compound as claimed in any of claims 1 to 3, wherein E6 is NH.
- 5. A process for preparing a compound as claimed in any of claims 1 to 4, which comprises reacting a compound of the formula IIa or IIb with a compound of the formula III to form a compound of the formula IVa or IVb (step a)) and subsequently reducing the compound of the formula IVa or IVb to give a compound of the formula Ia or Ib (step b)):

a)
$$E_4$$
 E_3 E_4 E_5 CHO

 H_2 E_6 E_1 E_2 or H_2 E_6 E_1 E_2 E_3 E_4 E_2 E_3 E_4 E_5 E_5 E_5 E_5 E_7 E_8 E_8

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where

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E1 is O, S, Se, Te, NR, CR₂, PR, preferably S.

E2, E3 are each CR, N, P,

E2', E3' are each O, S, Se, Te, NR, CR2, PR.

E4 is N, P, preferably N,

E5 is OH, SH, NHR, or OR', SR', NRR',

E6 is NH, PH, preferably NH, or NR', PR',

 R^5, R^6 are each hydrogen or a linear, branched or cyclic alkyl radical or an aryl radical,

R¹, R², R³, R⁴ are each hydrogen, a linear, branched or cyclic alkyl radical, an aryl radical, a halogen or a nitro group,

R is hydrogen, a linear, branched or cyclic alkyl radical,

R' is a linear, branched or cyclic alkyl radical, where at least one of the groups E5 and E6 contains a hydrogen atom.

- 6. The use of a compound as claimed in any of claims 1 to 4 for preparing metal complexes.
- 20 7. A metal complex of the formula V

 $L_xMR''_vY_z$ (V)

where

L is a monoanionic or dianionic ligand derived from a compound of the formula Ia or Ib as claimed in any of claims 1 to 4

where,

- in the case of a dianionic ligand,

E5 is O', S', RN', preferably O', and

E6 is N', P', preferably N',

30 and, in the case of a monoanionic ligand, either

> E5 is O', S', RN', preferably O', and

is NR, PR E6

or

35 E5 is OR, SR, NRR', and E6 is N, P, preferably N,

and the further symbols E1, E2, E2', E3, E3', E4, R⁵, R⁶, R¹, R², R³, R⁴, R and R' in the formulae I and II have the same meanings as forth for the corresponding symbols in any of claims 1 to 4;

and, when L is a dianionic ligand,

M is Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, preferably Ti, Zr, Hf,

R" is hydrogen, a hydrocarbon radical, preferably a linear, branched or cyclic alkyl radical, NR", OR", halogen, acetylacetonate, preferably halogen, OR", where R" is hydrogen or a linear, branched or cyclic alkyl radical,

Y is a Lewis acid,

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x is 1 or 2, preferably 1,

y is from 1 to 4, preferably 2,

z is from 0 to 2, preferably 0

where R" and Y may be joined to form a joint radical and 2x + y corresponds to the valence of M;

or, when L is a monoanionic ligand,

M is Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Ni, Pd, Co, Fe, Cu, Ru, Rh, preferably Ti, Zr, Hf, Ni, Pd,

R" is hydrogen, a hydrocarbon radical, preferably a linear, branched or cyclic alkyl radical, NR", OR", halogen, acetylacetonate, preferably halogen, OR", where R" is hydrogen or a linear, branched or cyclic alkyl radical,

Y is a Lewis acid,

x is 1, 2 or 3,

y is from 1 to 4,

z is from 0 to 2, preferably 0, where R'' and Y may be joined to form a joint radical and x + y corresponds to the valence of M.

- 8. A metal complex as claimed in claim 7, wherein the ligand L is a dianionic ligand and M is Ti, Zr or Hf.
- 9. A metal complex as claimed in claim 8, wherein x is 1, y is 2 and z is 0.
- 10. A metal complex as claimed in claim 7, wherein the ligand L is a monoanionic ligand and M is Ti, Zr, Hf, Ni or Pd.

A metal complex as claimed in claim 10, wherein when M is Ti, Zr, Hf, x is 2, y is 11. 2 and z is 0 or x is 1, y is 3 and z is 0 and when M is Ni or Pd, x is 1, y is 1 and z is 0.

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12. A process for preparing a metal complex as claimed in any of claims 7 to 11 by deprotonation of a compound as claimed in any of claims 1 to 4 by means of a base and subsequent reaction with a metal compound, or

by direct reaction of a compound as claimed in any of claims 1 to 4 with a metal compound,

where the metal compound comprises a metal M selected from the group consisting of Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W, preferably Ti, Zr, Hf, when L is a dianionic ligand, or a metal M selected from the group consisting of Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Ni, Pd, Co, Fe, Cu, Ru and Rh, preferably Ti, Zr, Hf, Ni, Pd, when L is a monoanionic ligand.

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- 13. A catalytically active composition comprising
 - a metal complex of the formula V as claimed in any of claims 7 to 11 as a) component A,

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- at least one compound, as component B, selected from the group consisting b) of
 - an organometallic compound, as component B1, (b1)
 - an organoaluminum oxy compound, as component B2, and (b2)

(b3) a compound which reacts with the metal complex to form an ion pair, as component B3.

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A catalytically active composition as claimed in claim 13 which further comprises a 14. support material (component C) in addition to the components A and B.

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A process for preparing a catalytically active composition as claimed in claim 13 or 15. 14, which comprises bringing a metal complex of the formula V as claimed in any of claims 7 to 11 (component A) into contact with a compound (component B) selected from the group consisting of

- (b1) an organometallic compound, as component B1,
- (b2) an organoaluminum oxy compound, as component B2, and
- (b3) a compound which reacts with the metal complex to form an ion pair, as component B3,
- and optionally a support material (component C).

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- 16. The use of a catalytically active composition as claimed in claim 13 or 14 for the polymerization or copolymerization of olefins.
- 17. A process for the polymerization or copolymerization of olefins, which comprises polymerizing an olefin in the presence of a catalytically active composition as claimed in claim 13 or 14 or copolymerizing at least two different olefins in the presence of a catalytically active composition as claimed in claim 13 or 14.
- 15 18. A polymer or copolymer which can be prepared by a process as claimed in claim 17.